

10/ 070,804

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated  
and searchable  
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in  
CA/CAPLUS  
NEWS 5 FEB 05 German (DE) application and patent publication number format  
changes  
NEWS 6 MAR 03 MEDLINE and LMedline reloaded  
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded  
NEWS 8 MAR 03 FRANCEPAT now available on STN  
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN  
NEWS 10 MAR 29 WPIFV now available on STN  
NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA  
NEWS 12 APR 26 PROMT: New display field available  
NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field  
available  
NEWS 14 APR 26 LITAlert now available on STN  
NEWS 15 APR 27 NLDB: New search and display fields available  
NEWS 16 May 10 PROUSDDR now available on STN  
NEWS 17 May 19 PROUSDDR: One FREE connect hour, per account, in both May  
and June 2004  
NEWS 18 May 12 EXTEND option available in structure searching  
NEWS 19 May 12 Polymer links for the POLYLINK command completed in REGISTRY  
NEWS 20 May 17 FRFULL now available on STN  
  
NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
specific topic.

All use of STN is subject to the provisions of the STN Customer  
agreement. Please note that this agreement limits use to scientific  
research. Use for software development or design or implementation  
of commercial gateways or other similar uses is prohibited and may  
result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 16:32:28 ON 18 MAY 2004

10/ 070,804

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:32:33 ON 18 MAY 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAY 2004 HIGHEST RN 682740-60-9

DICTIONARY FILE UPDATES: 17 MAY 2004 HIGHEST RN 682740-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

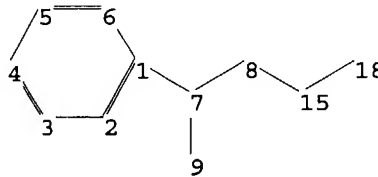
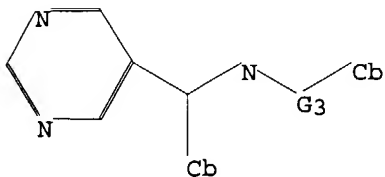
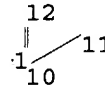
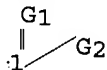
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\10070804.str



chain nodes :

7 8 9 10 11 12 15 18

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 7-8 7-9 8-15 10-11 10-12 15-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 8-15 10-11 10-12 15-18

exact bonds :

1-7 7-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:O,S

10/ 070,804

G2:O,S,N

G3:SO2, [\*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS  
11:CLASS 12:CLASS 15:CLASS 18:Atom

Generic attributes :

9:

Saturation : Unsaturated

18:

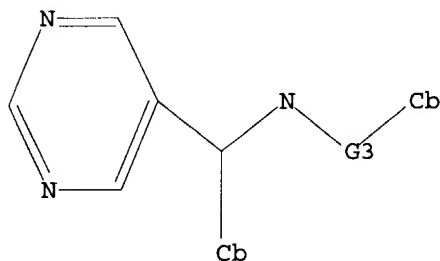
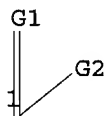
Saturation : Unsaturated

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 O,S,N

G3 SO2, [@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 16:33:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 25010 TO ITERATE

100.0% PROCESSED 25010 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

10/ 070,804

FULL ESTIMATED COST

155.42

155.63

FILE 'CAPLUS' ENTERED AT 16:33:09 ON 18 MAY 2004  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 18 May 2004 VOL 140 ISS 21  
FILE LAST UPDATED: 17 May 2004 (20040517/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2

L3 1 L2

=> d l3 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:765979 CAPLUS

DOCUMENT NUMBER: 132:46209

TITLE: A comparative molecular field analysis study of

obtusifoliol 14 $\alpha$ -methyl demethylase inhibitors

AUTHOR(S): Bargar, Tom M.; Secor, Jacob; Markley, Lowell D.;  
Shaw, Brian A.; Erickson, Jon A.

CORPORATE SOURCE: Dow AgroSciences, Indianapolis, IN, 46268, USA

SOURCE: Pesticide Science (1999), 55(11), 1059-1069

CODEN: PSSCBG; ISSN: 0031-613X

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This report describes the development of a Comparative Mol. Field Anal. (ComFA) model from a set of obtusifoliol 14 $\alpha$ -Me demethylase (DM) inhibitors to aid in the design of herbicides targeting sterol biosynthesis. ComFA is a three-dimensional (3-D) quant. structure-activity relationship (QSAR) method that is useful in the probing of receptor binding sites when exptl. structure data are unavailable. Conformational anal. and SAR of some rigid and active analogs were used to build the initial model using the active analog hypothesis. The model was subsequently used to design compds. that retain the active site shape requirements, but incorporate phys. properties that favor soil-applied herbicidal action. In addition, a second-generation ComFA model incorporating the newly designed inhibitors was developed and represents the current understanding of the DM binding site. This model was derived from a pharmacophore developed from two methods, the active analog approach as well as from the Catalyst program. The fact that two independent methods produced a similar pharmacophore strengthens the validity of the model.

IT 252895-58-2 252895-60-6

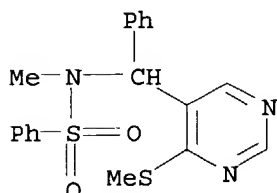
RL: AGR (Agricultural use); BAC (Biological activity or effector, except

10/ 070,804

adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL  
(Biological study); USES (Uses)  
(herbicidal obtusifolios 14 $\alpha$ -Me demethylase inhibitor, used in  
comparative mol. field anal. model)

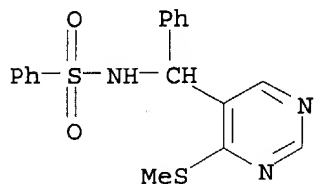
RN 252895-58-2 CAPLUS

CN Benzenesulfonamide, N-methyl-N-[[4-(methylthio)-5-  
pyrimidinyl]phenylmethyl]- (9CI) (CA INDEX NAME)



RN 252895-60-6 CAPLUS

CN Benzenesulfonamide, N-[[4-(methylthio)-5-pyrimidinyl]phenylmethyl]- (9CI)  
(CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 16:32:28 ON 18 MAY 2004)

FILE 'REGISTRY' ENTERED AT 16:32:33 ON 18 MAY 2004

L1 STRUCTURE UPLOADED

L2 2 S L1 FUL

FILE 'CAPLUS' ENTERED AT 16:33:09 ON 18 MAY 2004

L3 1 S L2

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.19	160.82

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.69	-0.69

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 16:33:40 ON 18 MAY 2004